Table S1 Locations of populations of four species sampled, number of each chlorotype and mitotype per population, and estimates of gene diversity for chlorotypes (H_C) and mitotypes (H_M) within populations.

						Chlorotype														Mitotype						
Population		Lat. (N)	Long. (E)	Alt. (m)	*N*	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	H_C	M1	M2	M3	M4	M5	M6	H_M
P. sylvestris var. *mongolica*																										
1#	Honghuaerji IM	48°05′	119°48′	904	12	11	0	0	0	0	0	1	0	0	0	0	0	0	0.17	12	0	0	0	0	0	0
2#	Hailaer IM	48°46′	119°43′	629	12	11	0	0	1	0	0	0	0	0	0	0	0	0	0.17	12	0	0	0	0	0	0
3#	Yakeshi IM	49°05′	121°10′	750	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
4#	Eerguna IM	51°17′	120°53′	823	12	10	0	2	0	0	0	0	0	0	0	0	0	0	0.30	12	0	0	0	0	0	0
5	Jinhezhen IM	50°57′	121°51′	760	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
6	Aokeliduishan IM	51°48′	121°59′	842	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
7	Genhe IM	51°48′	121°24′	742	12	11	1	0	0	0	0	0	0	0	0	0	0	0	0.17	12	0	0	0	0	0	0
8	Manguizhen IM	52°00′	121°46′	642	12	10	2	0	0	0	0	0	0	0	0	0	0	0	0.30	12	0	0	0	0	0	0
9	I-H bianjie	52°22′	122°08′	862	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
10	Chaohe HLJ	52°41′	122°39′	526	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
11	Mohe HLJ	53°03′	122°22′	496	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
12#	Amuerzhen HLJ	52°54′	123°07′	609	12	11	0	0	1	0	0	0	0	0	0	0	0	0	0.17	12	0	0	0	0	0	0
13	Tahe HLJ	52°42′	123°55′	424	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
14	Yongqing HLJ	52°26′	125°15′	317	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
15#	Xiushan HLJ	52°14′	124°41′	395	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
16	Jiagedaqi HLJ	51°37′	123°60′	627	12	11	0	0	1	0	0	0	0	0	0	0	0	0	0.17	12	0	0	0	0	0	0
17	Ganhe IM	50°48′	123°10′	610	12	10	1	1	0	0	0	0	0	0	0	0	0	0	0.32	12	0	0	0	0	0	0
18#	Neijiang HLJ	49°11′	125°32′	368	12	12	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0
19	Heihe HLJ	50°15′	127°30′	133	10	10	0	0	0	0	0	0	0	0	0	0	0	0	0	10	0	0	0	0	0	0
20	Jidong HLJ	45º06´	131º15´	180	8	7	0	0	0	0	1	0	0	0	0	0	0	0	0.25	8	0	0	0	0	0	0
21	Muling HLJ	44º54´	130º33´	277	8	7	0	0	0	0	1	0	0	0	0	0	0	0	0.25	8	0	0	0	0	0	0
22	Mulingzhen HLJ	44º31´	130º16´	373	5	5	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	1	0	0.40

23	Chaihe HLJ	44º45´	129º41´	310	8	7	0	0	0	1	0	0	0	0	0	0	0	0	0.25	7	0	0	0	0	1	0.25
Subtotal					255	241	4	3	3	1	2	1	0	0	0	0	0	0		253	0	0	0	1	1	
P. densiflora																										
24#	Jidong HLJ	45º06´	131º15´	180	8	0	1	0	0	0	0	0	7	0	0	0	0	0	0.25	0	0	8	0	0	0	0
25	Muling HLJ	44º54´	130º33´	277	8	1	0	0	0	0	0	0	5	1	1	0	0	0	0.64	0	0	8	0	0	0	0
26	Mulingzhen HLJ	44º31´	130º16´	373	11	3	0	0	0	0	0	0	8	0	0	0	0	0	0.44	0	0	11	0	0	0	0
27	Chaihe HLJ	44º45´	129º41´	310	8	2	0	0	0	0	0	0	6	0	0	0	0	0	0.43	0	0	8	0	0	0	0
28	Helong JL	42°24′	128°45′	564	16	1	0	0	0	0	0	0	15	0	0	0	0	0	0.13	0	0	16	0	0	0	0
29#	Changbai JL	41°26′	128°11′	1024	8	0	0	0	0	1	0	0	7	0	0	0	0	0	0.25	0	1	0	7	0	0	0.25
30	Linjiang JL	41º48´	126º54´	349	7	0	0	0	0	0	0	0	6	1	0	0	0	0	0.29	0	7	0	0	0	0	0
31#	Tonghua JL	41º45´	125º59´	392	7	0	0	0	0	0	0	0	6	1	0	0	0	0	0.29	0	4	0	3	0	0	0.57
32	Huanren LN	41º14´	125º23´	400	8	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	8	0	0	0	0	0
33#	Huanren LN	41º22´	124º56´	512	8	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	8	0	0	0	0	0
34	Benxi LN	41º16´	123º47´	508	6	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	6	0	0	0	0	0
35#	Fengcheng LN	40º25´	124º04´	176	8	0	0	0	0	0	0	0	7	0	0	1	0	0	0.25	0	8	0	0	0	0	0
36	Dandong LN	40º08´	124º22´	40	5	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	5	0	0	0	0	0
37	Zhuanghe LN	39º41´	122º57´	15	8	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	8	0	0	0	0	0
38	Dalian LN	38º47´	121º09´	29	8	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	8	0	0	0	0	0
39#	Yantai SD	37º17´	121º44´	104	11	0	0	0	0	0	0	0	9	2	0	0	0	0	0.33	0	11	0	0	0	0	0
40	Qingdao SD	36º07´	120º37´	16	5	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	5	0	0	0	0	0
41#	Lianyungang JS	34º38´	119º15´	126	8	0	0	0	0	0	0	0	7	1	0	0	0	0	0.25	0	8	0	0	0	0	0
Subtotal					148	7	1	0	0	1	0	0	131	6	1	1	0	0		0	87	51	10	0	0	
P. funebris																										
42#	Erdao JL	42°26′	128°07′	703	22	17	0	0	0	0	0	0	5	0	0	0	0	0	0.37	0	0	0	22	0	0	0
43#	Baihe JL	42°27′	128°08′	693	15	5	2	0	2	0	0	0	4	0	0	0	2	0	0.82	0	5	0	10	0	0	0.48
Subtotal					37	22	2	0	2	0	0	0	9	0	0	0	2	0		0	5	0	32	0	0	
P. takahasii																										
44#	Xingkaihu HLJ	45°18´	132°43´	72	17	11	0	0	0	0	0	0	6	0	0	0	0	0	0.49	0	1	16	0	0	0	0.12

45#	Xingkaihu HLJ	45º20´	132º23´	76	16	10	0	0	0	0	0	0	6	0	0	0	0	0	0.50	0	0	16	0	0	0	0
46	Mishan HLJ	45º30´	132º2´	152	8	1	0	0	0	0	0	0	5	1	0	0	0	1	0.68	0	0	8	0	0	0	0
47	Mishan HLJ	45º28´	131º42´	156	8	4	0	1	0	0	0	0	3	0	0	0	0	0	0.64	0	0	8	0	0	0	0
Subtotal					49	26	0	1	0	0	0	0	20	1	0	0	0	1		0	1	48	0	0	0	
Total					489	296	7	4	5	2	2	1	160	7	1	1	2	1		253	92	99	43	1	1	

Abbreviations after localities indicate provinces as follows: IM, Inner Mongolica; HLJ, Hei longjiang; JL, Jilin; LN, Liaoning; SD,Shandong; JS, Jiangsu. #, the populations which were also investigated by nuclear loci.

Table S2 Descriptions of the investigated eight nuclear loci.

Locus	Putative function	PCR primers (5'-3')	AT	Reference
a3ip2	ABI3-interacting protein 2	F: AATGCCAGGTTGGTGTTA R: CAGCCTCAATTTGCTTTCC	60	Wachowiak *et al.*, 2009
ccoaomt	Lignin biosynthesis	F: GCAGCAGAAGTGAAGGCTCAGA R: TCTTTCCATCATCGGGCAATG	58	Gonzalez-Martinez *et al.*, 2006
pod	Peroxidase	F: CCGATGCTGACTCTTCTAAC R: AGCGAATTTGGAGGATGA	55	Ma *et al.*, 2006
c3h-1	Coumarate 3-hydroxylase	F: AGCGAATTTGGAGGATGA R: TGGGTCCTTCCATACAGC	60	Brown *et al.*, 2004
CesA2	Cellulose synthase	F: AGATCTTGCTCAATGCCTCG R: CCAAACTTCACTGTCACATCG	58	Brown *et al.*, 2004
dhn1	Dehydrin 1 protein	F: TCACCGCACCCACAGTTC R: TCCGTCGGCTCACATTCA	60	Wachowiak *et al.*, 2009
erd3	Early responsive to dehydration 3	F: GAACGGGTCCGTACATTTTCTG R: TGCCAGATTGATTGGCATAGAA	60	Eveno *et al.*, 2008
aqua-MIP	Putative aquaporin	F: TGTCACTGCCCAGAGCTATTC R: ATCACAGCCGCTCCAAAAC	60	Gonzalez-Martinez *et al.*, 2006

AT, Annealing temperature.

Reference:

Brown GR, Gill GP, Kuntz RJ, Langley CH, Neale DB (2004). Nucleotide diversity and linkage disequilibrium in loblolly pine. *Proc Natl Acad Sci USA* **101**: 15255–15260.

Eveno E, Collada C, Guevara MA, Léger V, Soto A, Díaz L *et al.* (2008). Contrasting patterns of selection at *Pinus pinaster* Ait. drought stress candidate genes as revealed by genetic differentiation analyses. *Mol Biol Evol* **25**: 417–437.

Gonzalez-Martinez SC, Ersoz E, Brown GR, Wheeler NC, Neale DB (2006). DNA sequence variation and selection of tag single nucleotide polymorphisms at candidate genes for drought stress response in *Pinus taeda* L. Genetics **72**:1915–1926.

Ma XF, Szmidt, A.E., Wang XR. (2006). Genetic structure and evolutionary history of a diploid hybrid pine *Pinus densata* inferred from the nucleotide variation at seven gene loci. *Mol Biol Evol* **23**: 807-816.

Wachowiak W, Balk PA, Savolainen O (2009). Search for nucleotide diversity patterns of local adaptation in dehydrins and other cold-related candidate genes in Scots pine (Pinus sylvestris L). *Trees Genet Genomes* **5**: 117–132.

Table S3 The variable sites in aligned cpDNA and mtDNA sequences which gave rise to thirteen chlorotypes and six mitotypes recorded across the four pine species.

	Nucleotide variable positions											
	*rpl*16			*trn*S-*trn*G				*rbc*L				
Chlorotype	149	165	662	12	200	234	517	709	731	765	1199	1315
C1	-	*	G	§	A	A	C	A	T	T	T	T
C2	-	*	T	§	A	A	C	A	T	T	T	T
C3	-	*	G	§	G	A	C	A	T	T	T	T
C4	-	*	G	§	A	C	C	A	T	T	T	T
C5	-	*	G	-	A	A	C	A	T	T	T	T
C6	-	*	G	§	A	A	C	G	T	T	T	G
C7	-	*	G	§	A	A	C	A	T	G	T	T
C8	-	*	G	§	A	A	C	G	C	T	C	T
C9	-	*	G	-	A	A	C	G	C	T	C	T
C10	-	*	G	§	A	A	T	G	C	T	C	T
C11	#	*	G	§	A	A	C	G	C	T	C	T
C12	-	*	T	-	A	A	C	A	T	T	T	T
C13	-	-	G	§	A	A	C	G	C	T	C	T

	Nucleotide variable positions																					
	*nad*5							*nad*4/3-4			*nad1* exon *B/C*								*nad7* intron *1*			
Mitotype	192	269	273	340	344	462	595	164	280	284	781	822	825	886	894	919	1111	1287	546	549	675	850
M1	G	-		-		A	A	□	-		□	C	○	C	G	C	□	■	C	□	-	C

M2	-	ATGGC	TGGGT	C	C	▲	TGCTC	-	A	●	-	-	C	▼	-	A	□	□	C
M3	-	ATGGC	TGGGT	C	C	▲	TGCTC	-	A	●	-	-	C	▼	-	A	□	□	A
M4	-	ATGGC	TGGGT	C	C	▲	TGCTC	-	A	●	-	-	A	▼	-	A	□	□	C
M5	G	-	-	A	A	□	-	-	A	●	-	-	C	▼	-	C	□	-	C
M6	G	-	-	A	A	□	-	-	A	●	-	-	A	▼	-	C	□	-	C

Dashes indicate missing nucleotides. **#** ATATTTTGATCTAATG, ***** ATAT, **§** CAG

▲ ATTGGGTGGGGGGGCTTATGGT

□CTTTTTTACTTACTTTAGAGGATGCGTAAGCACGCTCGACTGTTAAGGAGAGGGGCAAATAAGTCAAAAAAAGGGT

● GGCCTCC

○ TTTTACTTACTTTAGAGGATGCGTAAGCACGCTCGACTGTTAAGGAGAGGGG

▼ GGGGGTCGAGCGTT

□TCTTCGCGTTCCTCTCTTTTGGGGCCCCTCCCCCAAAAGAGAGTTGTTCGTCTCCTCACA

□ GGGTGGCCCCTCTC

□ TTTTTTTTACTTATTTGGGGGATGCGTAAGCAGGCTCGACTGTTAAGGAGAGGGGC

□ CCGGAGGGCTTGCGCTTCTGAGGGCAAGGT

□GATGGCGGCCCTCTCCTTAACAGTCGAGTACCTAAAGGTCCTTATGGTCGAGTACCTAAAGGT

■CTCCTCTCCCTTGGGGTCGAGTACCTAAAGGTCCTTATCAGTCGAGCCCCCTAAAGGGTCCT

Table S4 Estimates of average genetic diversity within populations (H_S), total genetic diversity (H_T), interpopulation differentiation (G_{ST}), and the number of substitution types (N_{ST}) (mean ± SE in parentheses) for haplotypes (*P. funebris*: not estimated due to less than three populations).

Regions	H_S	H_T	G_{ST}	N_{ST}
Chlorotype				
Four species	0.199 (0.031)	0.562 (0.025)	0.645 (0.050)	0.745 (0.048)*
P. sylvestris var. *mongolica*	0.109 (0.026)	0.109 (0.025)	-0.000 (NC)	0.014(NC)
P. densiflora	0.196 (0.045)	0.201 (0.045)	0.024 (NC)	0.032 (NC)
P. takahasii	0.535 (0.073)	0.607 (0.082)	0.119 (0.019)	0.226 (0.150)*
P. funebris	–	–	–	–
Mitotype				
Four species	0.045 (0.019)	0.668 (0.044)	0.933 (0.028)	0.976 (0.015)*
P. sylvestris var. *mongolica*	0.028 (0.020)	0.028 (0.020)	-0.004 (NC)	-0.006 (NC)
P. densiflora	0.046 (0.034)	0.522 (0.090)	0.913 (0.062)	0.919 (0.055)
P. takahasii	0.029 (0.029)	0.029 (0.029)	-0.000 (NC)	0.000 (NC)
P. funebris	–	–	–	–

Table S5 Analysis of molecular variance (AMOVA) of cpDNA and mtDNA variation in four species.

Source of variation	d. F.	SS	VC	Variation (%)	Fixation index
Chlorotype					
Among all species	3	249.86	0.820	77.08	$F_{\mathrm{CT}} = 0.771^{***}$
Among populations within species	43	12.90	0.006	0.58	$F_{\mathrm{SC}} = 0.025^{*}$
Within populations	442	105.02	0.238	22.34	$F_{\mathrm{ST}} = 0.777^{***}$
Total	488	367.78	1.064		
Among populations within *P. sylvestris* var. *mongolica*	22	1.70	0.001	2.39	$F_{\mathrm{ST}} = 0.024^{*}$
Within populations	232	14.13	0.061	97.61	
Total	254	15.83	0.063		
Among populations within *P. densiflora*	17	4.67	0.005	2.13	$F_{\mathrm{ST}} = 0.021$
Within populations	130	30.33	0.233	97.87	
Total	147	35.00	0.238		
Between *P. sylvestris* var. *mongolica* and *P. densiflora*	1	246.67	1.316	91.20	$F_{\mathrm{CT}} = 0.912^{***}$
Among populations within species	39	6.38	0.004	0.29	$F_{\mathrm{SC}} = 0.033$
Within populations	342	44.46	0.123	8.51	$F_{\mathrm{ST}} = 0.915^{***}$
Total	402	297.51	1.443		
Mitotype					
Among all species	3	2112.60	6.947	97.55	$F_{\mathrm{CT}} = 0.976^{***}$
Among populations within species	43	45.49	0.097	1.36	$F_{\mathrm{SC}} = 0.555^{***}$
Within populations	442	34.34	0.078	1.09	$F_{\mathrm{ST}} = 0.989^{***}$
Total	488	2192.43	7.122		
Among populations within *P. sylvestris* var. *mongolica*	22	2.29	0.005	7.62	$F_{\mathrm{ST}} = 0.076^{*}$
Within populations	232	12.60	0.054	92.38	
Total	254	14.89	0.059		

Among populations within *P. densiflora*	17	42.17	0.287	68.10	$F_{ST} = 0.681^{***}$
Within populations	130	17.46	0.134	31.90	
Total	147	59.64	0.421		
Between *P. sylvestris* var. *mongolica* and *P. densiflora*	1	1571.90	8.387	97.78	$F_{CT} = 0.978^{***}$
Among populations within species	39	44.46	0.108	1.26	$F_{SC} = 0.565^{***}$
Within populations	362	30.06	0.083	0.97	$F_{ST} = 0.990^{***}$
Total	402	1646.42	8.578		

d.f., degrees of freedom; SS, sum of squares; VC, variance components;

$^{*}P<0.05$, $^{**}P<0.01$ and $^{***}P<0.001$, 1000 permutations.

F_{CT}, differentiation among groups within four species;

F_{SC}, differentiation among populations within species;

F_{ST}, differentiation among populations within four species

Table S6 Nucleotide variation at eight nuclear loci in (a) *P. slvestris* var. *mongolica*, (b) *P. densiflora*, (c) *P. funebris* and (d) *P. takahasii*.

		Total							Nonsynonymous sites				Silent sites			
Species	Locus	n	*L*	N_h (Indels)	*S*	θ_{wt}	πt	R_m	*L*	*S*	θ_{wa}	π_a	*L*	*S*	θ_{ws}	π_s
a	*a3ip2*	26	948	7	10	0.00283	0.00325	0	143.5	0	0	0	780.5	10	0.00336	0.00386
	ccoaomt	26	502	2	5	0.00261	0.00091	0	197	0	0	0	305	5	0.0043	0.00149
	pod	24	365	6	10	0.00738	0.0093	0	88.69	0	0	0	274.31	10	0.00976	0.01231
	c3h-1	27	676	5	8	0.0031	0.00287	0	245.44	1	0.00106	0.00146	422.56	7	0.0043	0.0037
	CesA2	21	516	2	7	0.00377	0.00129	0	286.33	0	0	0	229.67	7	0.00847	0.0029
	dhn1	23	1076	13	53	0.01632	0.01536	5	393.44	NA	NA	0.00556	516.56	NA	NA	0.02212
	erd3	24	774	7	8	0.00277	0.00272	1	428.28	3	0.00188	0.0018	342.72	5	0.00391	0.00364
	aqua-MIP	13	560	3	11	0.00633	0.00568	0	148.67	0	0	0	411.33	11	0.00862	0.00773
	Total	_	5417	45	112	_	_	6	1931.35	4	_	_	3282.65	44	_	_
	Average	23	677.13	5.625	14	0.00627	0.00579	0.75	241.42	0.57	0.00069	0.00172	410.33	7.8571	0.00552	0.00759
b	*a3ip2*	22	948	3	0	0	0	NA	143.5	0	0	0	710.5	0	0	0
	ccoaomt	23	502	9	7	0.00379	0.0021	0	197	1	0.00138	0.00044	304	6	0.00535	0.00317
	pod	17	365	8	18	0.01471	0.01334	2	88.67	1	0.00334	0.00133	274.33	18	0.01948	0.01724
	c3h-1	25	676	9	14	0.00558	0.00358	2	245.74	1	0.00108	0.00155	417.26	13	0.00825	0.00479
	CesA2	26	516	6	5	0.00254	0.00265	0	286.32	0	0	0	229.68	5	0.0057	0.00595
	dhn1	18	1117	13	47	0.0149	0.01572	7	400.81	NA	NA	0.00788	516.19	NA	NA	0.02182
	erd3	27	774	8	7	0.00235	0.00169	1	428.4	2	0.00121	0.00145	342.6	5	0.00379	0.00201
	aqua-MIP	20	560	13	15	0.00755	0.00695	4	148.67	0	0	0	411.33	15	0.01028	0.00947
	Total	_	5458	61	113	_	_	16	1939.11	5	_	_	3205.89	47	_	_
	Average	22.25	682.25	8.625	14.13	0.00642	0.00595	2.29	242.39	0.63	0.00088	0.00225	400.74	8.86	0.00641	0.00777
c	*a3ip2*	10	948	5	10	0.00404	0.00432	0	143.5	0	0	0	728.5	10	0.00485	0.00519
	ccoaomt	11	502	6	9	0.00613	0.00581	0	197	0	0	0	304	9	0.01011	0.00957
	pod	9	365	3	10	0.01014	0.01377	0	88.67	0	0	0	274.33	10	0.01341	0.01823

	c3h-1	12	676	5	9	0.00449	0.00541	0	245.42	1	0.00135	0.00123	417.58	8	0.00634	0.00787
	CesA2	11	516	6	4	0.00265	0.00324	1	286.21	0	0	0	229.79	4	0.00594	0.00728
	dhn1	7	1069	5	37	0.01643	0.01383	4	400.45	NA	NA	0.0063	518.55	NA	NA	0.01965
	erd3	11	774	4	8	0.00353	0.00366	0	428.38	4	0.00319	0.00246	342.62	4	0.00399	0.0052
	aqua-MIP	11	560	8	17	0.01036	0.01026	2	148.67	0	0	0	411.33	17	0.01411	0.01397
	Total	_	5410	42	104	_	_	7	1938.3	5	_	_	3226.7	45	_	_
	Average	10.25	676.25	5.25	13	0.007598	0.00753	0.88	242.29	0.71	0.0011	0.002001	403.34	8.86	0.00793	0.01065
d	*a3ip2*	8	948	3	11	0.00485	0.00499	0	143.5	0	0	0	728.5	11	0.00582	0.00598
	ccoaomt	9	502	6	8	0.00588	0.0061	0	197	0	0	0	304	8	0.00968	0.01005
	pod	8	365	7	11	0.01169	0.01328	2	88.67	1	0.00435	0.00604	274.33	10	0.01406	0.01562
	c3h-1	8	676	5	10	0.00581	0.00737	2	245.58	1	0.00157	0.00233	417.42	9	0.00832	0.01035
	CesA2	9	516	3	3	0.00214	0.00258	0	286.33	0	0	0	229.67	3	0.00481	0.00581
	dhn1	7	1085	4	32	0.01375	0.01519	3	400.98	9	0.00916	0.00962	549.02	25	0.01859	0.01925
	erd3	10	774	6	8	0.00365	0.00388	0	428.27	4	0.0033	0.00311	342.73	4	0.00413	0.00486
	aqua-MIP	7	560	6	15	0.01093	0.00969	2	148.67	0	0	0	411.33	15	0.01488	0.0132
	Total	_	5426	40	98	_	_	9	1939	15	_	_	3257	85	_	_
	Average	8.25	678.25	5	12.25	0.007503	0.00808	1.13	242.38	1.88	0.00302	0.003245	407.13	10.63	0.01024	0.01075

n, sample size; *L*, length in base pairs; *S*, number of segregating sites; π, nucleotide diversity; θ_w, Watterson's parameter; R_m, the minimum number of recombinant events; NA: failed to be computed for lack of enough variation. The average values of all θ_w and π here are weighted average values. N_h (Indels), number of haplotypes with indels included.

Table S7 Migration rates among the four species implemented in Lamarc 2.1.5.

Migration rates (*M*)	*P. sylvestris* var. *mongolica*	*P. densiflora*	*P. funebris*	*P. takahasii*
>*P. sylvestris* var. *mongolica*	-	321	473	257
>*P. densiflora*	158	-	354	352
>*P. funebris*	378	619	-	273
>*P. takahasii*	269	573	482	-

>, migrate into the species.

Table S8 The prior distributions of parameters used for description of the scenarios analysed in DIYABC v1.0.4.39 (Cornuet et al. 2010).

As the prior distributions of parameters often overlapped, several conditions were considered. They were t4 > t1, t3 ≥ t2 and t2 > t1.

Parameter	Origin of *P. funebris*			Origin of *P. takahasii*		
	Distribution	Min.	Max.	Distribution	Min.	Max.
Effective population size						
N1(*P. sylvestris* var. *mongolica*)	uniform	10	1000000	uniform	10	1000000
N2(*P. densiflora*)	uniform	10	1000000	uniform	10	1000000
N3(*P. funebris*)	uniform	10	500000	_	_	_
N4(*P. takahasii*)	_	_	_	uniform	10	500000
Nm(*P. sylvestris* var. *mongolica*)	uniform	10	300000	uniform	10	300000
Nd(*P. densiflora*)	uniform	10	300000	uniform	10	300000
NA	uniform	10	500000	uniform	10	500000
Time of events						
t1	uniform	1	3000	uniform	1	3000
t2	uniform	1	10000	uniform	1	10000
t3	uniform	1	10000	uniform	1	10000
t4	uniform	1	100000	uniform	1	200000
Admixture rate						
r1/r2	uniform	0.001	0.999	uniform	0.001	0.999
Mean mutation rate	uniform	10^{-7}	10^{-9}	uniform	10^{-7}	10^{-9}

Table S9 Estimations of the posterior distributions of parameters revealed from the Approximate Bayesian Computation for the best scenario for origin of *P. funebris* (scenario 1.1 in Table 6). The estimation is based on 1% of the closest simulated datasets and the logit transformation of parameters was used.

Parameter	mean	median	mode	95% CI
N1	530000	519000	293000	109000-977000
N2	574000	596000	973000	84600-982000
N3	239000	229000	123000	21800-486000
Nm	86400	68300	40900	10600-260000
Nd	116000	99800	57700	14600-279000
NA	128000	98100	49600	14200-408000
t1(kya)	35	33	9	2-73
t2(kya)	114	110	90	23-220
t3(kya)	180	190	247	68-248
t4(kya)	1740	1850	2438	445-2470
r1	0.345	0.318	0.267	0.0313-0.831

kya, thousand years ago.

Table S10 Estimations of the posterior distributions of parameters revealed from the Approximate Bayesian Computation for the best scenario for origin of *P. takahasii* (scenario 2.1 in Table 6). The estimation is based on 1% of the closest simulated datasets and the logit transformation of parameters was used.

Parameter	mean	median	mode	95% CI
N1	522000	506000	389000	106000-971000
N2	563000	582000	993000	74800-984000
N4	254000	250000	111000	29300-488000
Nm	95200	79100	62300	13600-266000
Nd	112000	96000	59900	17100-275000
NA	124000	98100	67900	12800-390000
t1(kya)	36	35	12	2-73
t2(kya)	115	112	92	23-220
t3(kya)	179	189	245	64-247
t4(kya)	1735	1845	2353	443-2470
r2	0.202	0.169	0.155	0.0221-0.600

kya, thousand years ago.

Figure S1 Schemes of the same six scenarios for origin of *P. funebris* and *P. takahasii*. Effective population sizes are marked in different colours and in the left, times of events (not to scale) are in the right. For the parameter codes see Table S7.

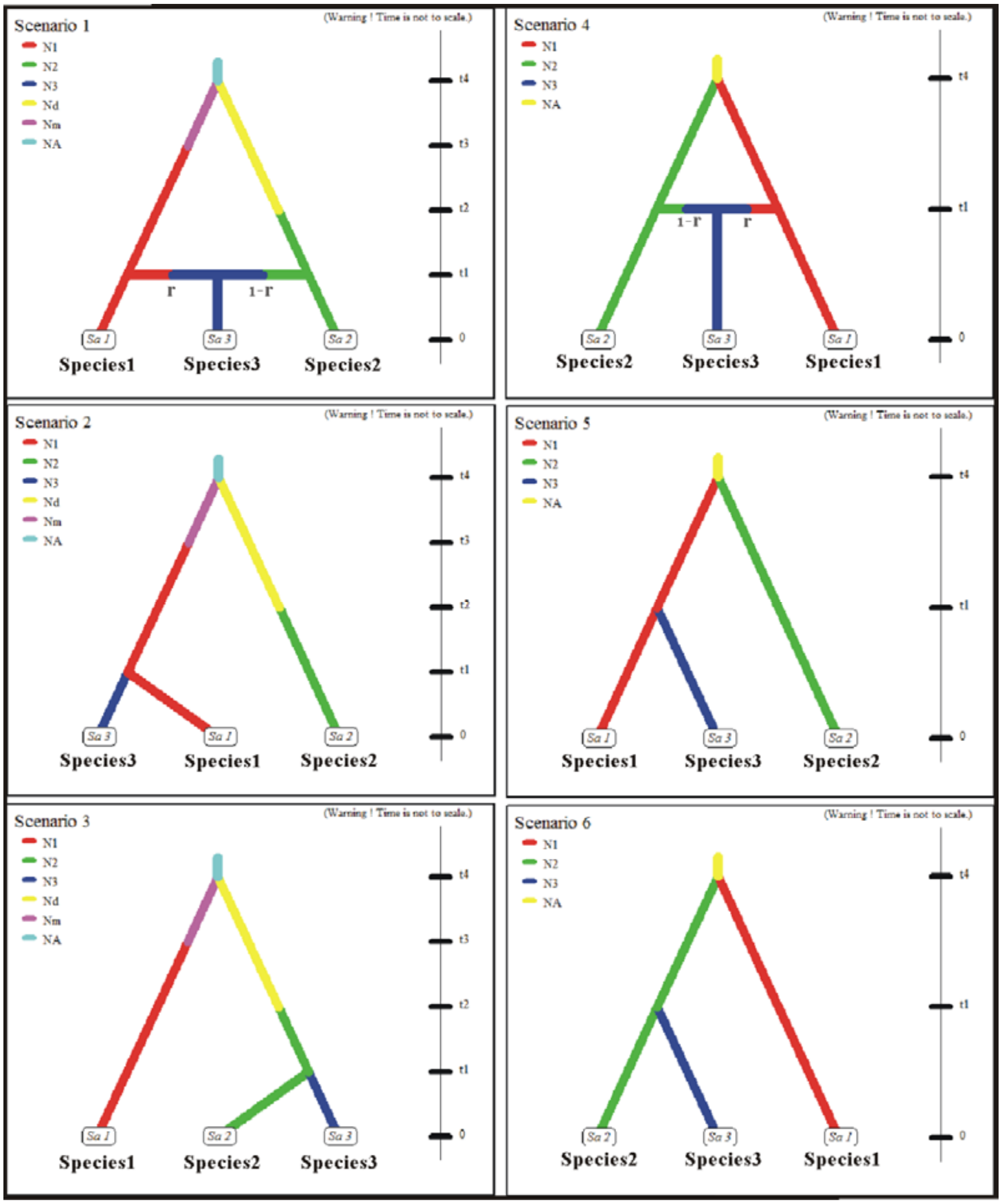

Figure S2 Structure analysis of (a) *P. slvestris* var. *mongolica*, (b) *P. funebris*, (c) *P. takahasii* and (d) *P. densiflora* when *K* =2–6 clusters are assumed. For each *K* value, results of the run with the highest value of LnPD were used.

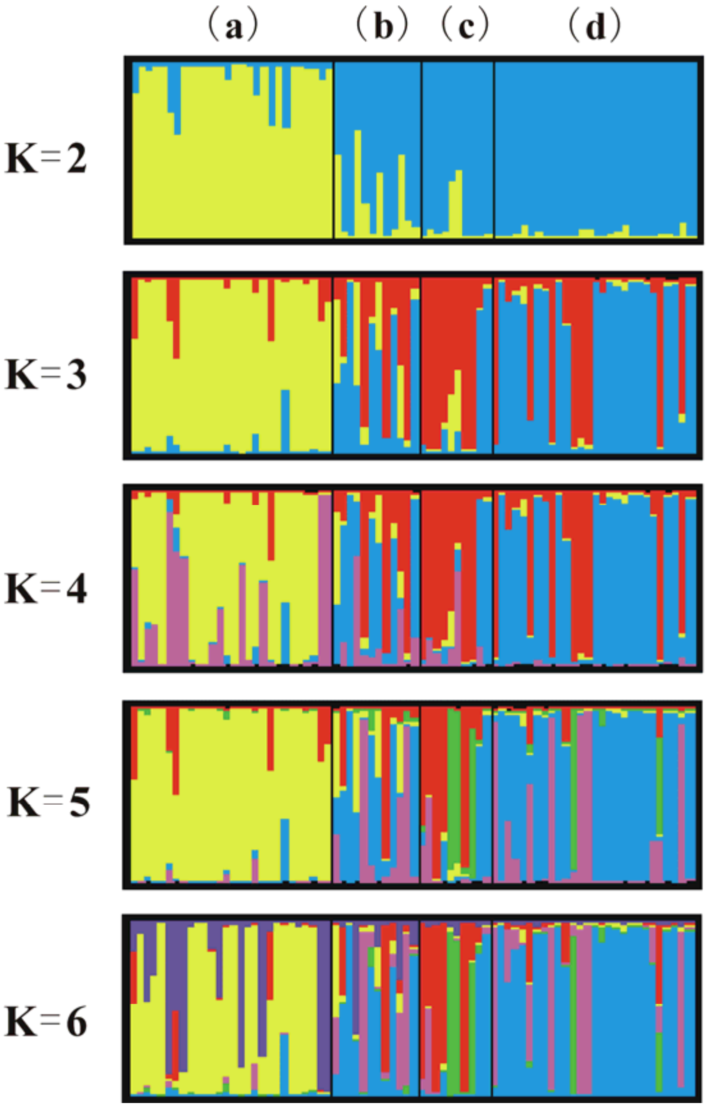

Figure S3 Comparison of the relative posterior probabilities for scenarios separately for either of two origins. They are computed via the logistic regression in DIYABC v1.0.4.39 on 1% of simulated datasets closest to the observed data.

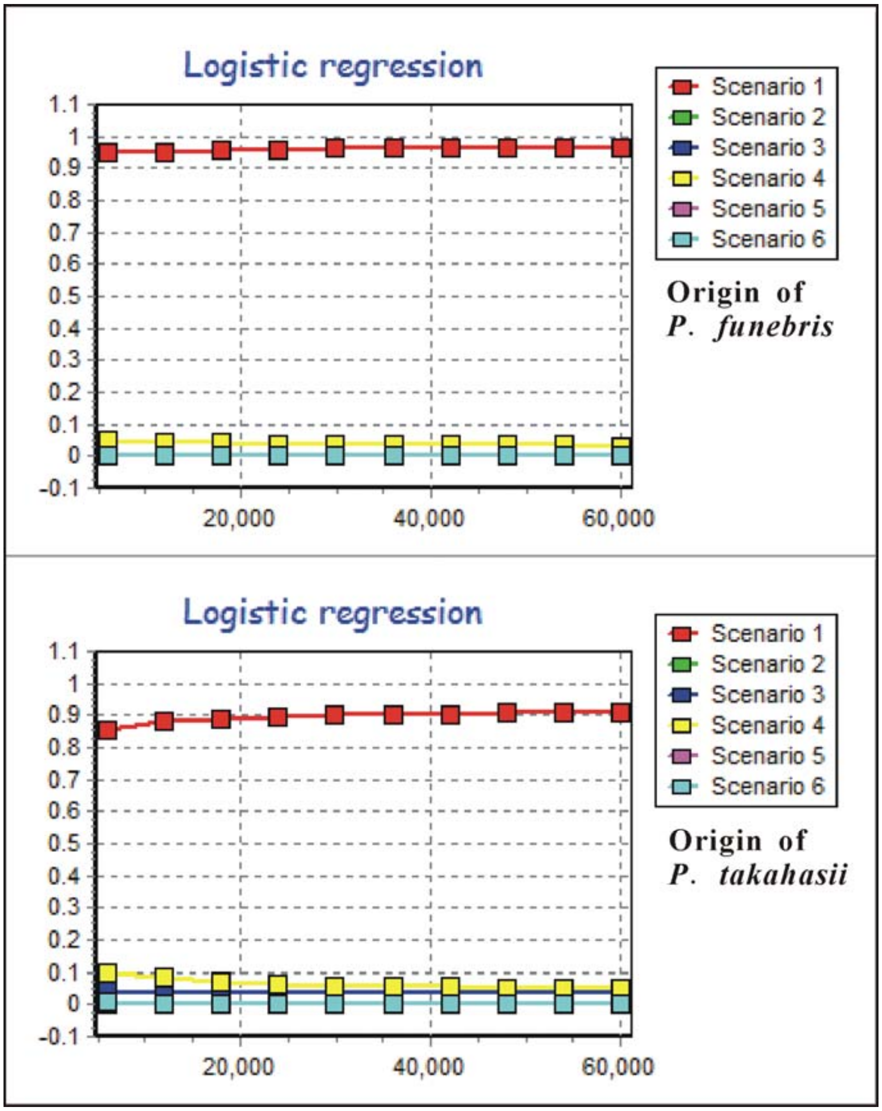

Figure S4 Illustration explaining the scenario of the homoploid hybrid speciation as a result of range shifts. (a) Range contract to different refugia, (b) range expansion and secondary contact of *P. sylvestris* var. *mongolica* and *P. densiflora* which were indicated by the dark and light gray, respectively, (c) hybridizations between *P. sylvestris* var. *mongolica* and two different refugia of*P. densiflora*, and subsequent formation of two hybrid species, *P. funebris* and *P. takahasii*(oval area).